

Phosphorodichloridothioic acid, O-methyl ester

Other names:	Dichloromethoxyphosphine sulfide Methyl dichlorothionophosphate Methyl dichlorothiophosphate O-Methyl phosphorodichloridothioate O-Methyl phosphorodichlorothioate Phosphorodichloridothioic acid, methyl ester O-Methyl dichlorothiophosphate Methyldichlorthiofosfat O-Methylester kyseliny dichlorthiofosforecne
Inchi:	InChI=1S/CH3Cl2OPS/c1-4-5(2,3)6/h1H3
InchiKey:	BJTWJPDCJVKDBK-UHFFFAOYSA-N
Formula:	CH3Cl2OPS
SMILES:	COP(=S)(Cl)Cl
Mol. weight [g/mol]:	164.98
CAS:	2523-94-6

Physical Properties

Property code	Value	Unit	Source
ie	9.85	eV	NIST Webbook
log10ws	2.11		Crippen Method
logp	2.335		Crippen Method
mcvol	92.110	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2523946&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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